Technical note (not for publication as it is)

Note on "From Quantum Dynamics to the Canonical Distribution – A Rigorous Derivation in Special Models"

Hal Tasaki[1]

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[1] Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, JAPAN
electronic address: hal.tasaki@gakushuin.ac.jp

1 About this note

This is a note associated with my paper "From Quantum Dynamics to the Canonical Distribution – A Rigorous Derivation in Special Models" (cond-mat/9707253). Here I describe all the technical details which are not discussed in the main paper.

Please note that this is not (yet) written as a regular paper. I did not include any introductory materials or physical discussions. The proofs may not be optimally organized yet.

The preset note is organized as follows. In Section 2, we prove a simple claim about the robustness of the non-resonance condition that we mentioned in the main paper. In Section 3, we prove the Theorem in the main paper. The theorem is essentially an application of the Chebysehv's inequality, and the proof is easy. In Section 4, we prove the Lemma in the main paper. As is clear from the table of contents, this is the hardest and the most technical part in our analysis. We have summarized the basic strategy in the beginning of the section. Section 5 is independent from the rigorous example we discuss in the main paper and in the present note. Here we deal with much more general class of models, and show that the "half" of the "hypothesis of equal weights for eigenstates" can be proved rather easily.

2 Non-resonance condition

Let us prove the statement about robustness of the non-resonance condition mentioned in the footnote [8] of the main paper.

Let E_i be an eigenvalue of H and let the corresponding normalized eigenstate be

$$\Phi_{E_i} = \sum_{j=1}^{n} \sum_{k=1}^{N} \varphi^{(i)}_{(j,k)} \Psi_j \otimes \Gamma_k. \tag{2.1}$$

From the first order perturbation theory, we get

$$\frac{\partial E_i}{\partial B_{k'}} = \sum_{j=1}^{n} |\varphi^{(i)}_{(j,k')}|^2. \tag{2.2}$$

Suppose that the energy spectrum $\{E_i\}$ violates the non-resonance condition for some E_i's in the range $E_i \geq \varepsilon_n + 2\lambda$. More precisely, we assume that there are i_1, i_2, i_3, i_4 such that $R = E_{i_1} - E_{i_2} - (E_{i_3} - E_{i_4}) = 0$ holds.

We now shift all the $B_{k'}$'s in the lowest band $(0, \delta)$ by a small amount, say d, keeping their spacing unchanged. If

$$\frac{\partial R}{\partial d} = \frac{\partial E_1}{\partial d} - \frac{\partial E_2}{\partial d} - \frac{\partial E_3}{\partial d} + \frac{\partial E_4}{\partial d} \tag{2.3}$$

is nonvanishing, then we can conclude that the resonance is lifted for any small shift d. Also note that no new resonances are generated if we keep d sufficiently small.

Let us assume that $\frac{\partial R}{\partial d}$ happens to be vanishing. In such a (extremely rare) situation, we shift all the $B_{k'}$'s in the second band $(\delta, 2\delta)$ by d'. We can then say that

$$\frac{\partial R}{\partial d'} = \frac{\partial E_1}{\partial d'} - \frac{\partial E_2}{\partial d'} - \frac{\partial E_3}{\partial d'} + \frac{\partial E_4}{\partial d'} \tag{2.4}$$

is nonvanishing. To see this we recall the representation (2.2). That $\frac{\partial R}{\partial d} = 0$ means that there is a very special relation between $\sum_{k';\text{lowest}} \sum_{j=1}^{n} |\varphi_{(j,k')}^{(i_\mu)}|^2$ with $\mu = 1, 2, 3, 4$. Since $\varphi_{(j,k)}$ is determined as the solution of the Schrödinger equation (4) in the main paper, it has different decay properties in the "classically inaccessible regions" for different values of E. This means that $\sum_{k';\text{second}} \sum_{j=1}^{n} |\varphi_{(j,k')}^{(i_\mu)}|^2$ with $\mu = 1, 2, 3, 4$ cannot satisfy the same special relation as the corresponding quantities of the lowest band. So we conclude that the resonance is lifted by a small d'.

The same argument works for the cases with multiple resonances. We see that all the resonances go away if we allow small d and d'.

3 Proof of Theorem

Let us prove the Theorem in the main paper. We first state and prove a general lemma, on which the desired theorem relies. Let $\Phi_{E'}$ be the eigenstate of the total Hamiltonian H with the eigenvalue E'. We assume that the initial state $\Phi(0)$ of the system is expanded as

$$\Phi(0) = \sum_{E'} \gamma_{E'} \Phi_{E'}, \tag{3.1}$$

and set

$$\bar{\gamma} = \max_{E'} |\gamma_{E'}|. \tag{3.2}$$

As in the main paper $\langle A \rangle_t$ denote the expectation value of the operator A of the subsystem in the state at time t. We have shown in the main paper that

$$\overline{\left\{ \langle A \rangle_t - \overline{\langle A \rangle_t} \right\}^2} \le n^2 (\|A\|_\infty)^2 \bar{\gamma}^2. \tag{3.3}$$

Then we have

Lemma 1 *Let A be an arbitrary operator of the subsystem. Let $\kappa > 0$ and $\Delta > 0$ be arbitrary constants. Then there exists a (κ-dependent) constant $T > 0$, and we have*

$$\frac{\tau_\Delta(T)}{T} \le \frac{(1+\kappa) n^2 (\|A\|_\infty)^2 \bar{\gamma}^2}{\Delta^2}, \tag{3.4}$$

where $\tau_\Delta(T)$ is the total length of the intervals within $0 \le t \le T$ at which

$$|\langle A \rangle_t - \overline{\langle A \rangle_t}| \ge \Delta \tag{3.5}$$

holds.

Proof: This is nothing but the Chebyshev's inequality, but we give a proof for completeness. For a function $f(t)$ of t, we let

$$v_T[f(t)] = \frac{1}{T} \int_0^T dt (f(t) - \overline{f(t)})^2. \tag{3.6}$$

Since (3.3) implies

$$\lim_{T\uparrow\infty} \upsilon_T[\langle A\rangle_t] \leq n^2(\|A\|_\infty)^2\bar{\gamma}^2, \tag{3.7}$$

we see from continuity that for a given $\kappa > 0$, there is $T > 0$ such that

$$\upsilon_T[\langle A\rangle_t] \leq (1+\kappa)n^2(\|A\|_\infty)^2\bar{\gamma}^2. \tag{3.8}$$

Now observe that

$$\chi\left[\left|\langle A\rangle_t - \overline{\langle A\rangle_t}\right| \geq \Delta\right] \leq \frac{\left(\langle A\rangle_t - \overline{\langle A\rangle_t}\right)^2}{\Delta^2}, \tag{3.9}$$

where the characteristic function χ is defined by $\chi[\text{true}] = 1$ and $\chi[\text{false}] = 0$. By averaging (3.9) over t such that $0 \leq t \leq T$, we find

$$\tau_\Delta(T) \leq \frac{\upsilon_T[\langle A\rangle_t]}{\Delta^2}, \tag{3.10}$$

which with (3.8) implies the desired (3.4). ■

In order to prove the Theorem in the main paper, we have to evaluate $\bar{\gamma}$ and choose appropriate Δ.

We recall that we have the initial state of the form

$$\Phi(0) = \Psi_n \otimes \sum_k \alpha_k \Gamma_k, \tag{3.11}$$

with α_k nonvanishing only for k such that

$$|E - (\varepsilon_n + B_k)| \leq \frac{\varepsilon_n}{2}, \tag{3.12}$$

for a fixed E such that $\varepsilon_n + 3\lambda \leq E \leq B_{\max} - 3\lambda$. To evaluate $\bar{\gamma}$, we note that

$$\gamma_{E'} = \langle \Phi_{E'}, \Phi(0)\rangle = \sum_k \overline{\varphi_{(n,k)}}\alpha_k, \tag{3.13}$$

where we wrote

$$\Phi_{E'} = \sum_{j=1}^{n}\sum_{k=1}^{N} \varphi_{(j,k)}\Psi_j \otimes \Gamma_k. \tag{3.14}$$

We shall prove in Section 4.6 that $|\varphi_{(n,k)}|$ is less than $O(\exp[-\text{const}.L^{1/3}])$ outside the interval $\{k_{\min}, \ldots, k_{\max}\}$ determined by the condition

$$|E' - (\varepsilon_n + B_j)| \leq \lambda + \text{const}.L^{-1/3}. \tag{3.15}$$

For E' such that $|E' - E| \geq \lambda + (\varepsilon_n/2)$, the two ranges (3.12), (3.15) have no overlaps, and we see that $|\gamma_{E'}|$ is small.

So we assume $|E' - E| \leq \lambda + (\varepsilon_n/2)$. From (3.13), we have

$$|\gamma_{E'}| \leq (\max_k |\alpha_k|) \sum_k |\varphi_{(n,k)}|. \tag{3.16}$$

By using the above observation about $|\varphi_{(n,k)}|$, we find

$$\begin{aligned}
\sum_k |\varphi_{(n,k)}| &\le \sum_{k=k_{\min}}^{k_{\max}} |\varphi_{(n,k)}| + \text{const.}\exp[-\text{const.}L^{1/3}] \\
&\le \left\{ \left(\sum_k |\varphi_{(n,k)}|^2 \right) \left(\sum_{k=k_{\min}}^{k_{\max}} 1 \right) \right\}^{1/2} + \text{const.}\exp[-\text{const.}L^{1/3}] \\
&\le (k_{\max} - k_{\min})^{1/2} + \text{const.}\exp[-\text{const.}L^{1/3}] \\
&\le \sqrt{2\lambda\rho(E' - \varepsilon_n + \lambda)} + \text{const.}\exp[-\text{const.}L^{1/3}] \\
&\le \sqrt{2\lambda\rho(E)}. \qquad (3.17)
\end{aligned}$$

By using the assume bound for α_k (see the main paper), we find that

$$|\gamma_{E'}|^2 \le \frac{2c'\lambda}{\varepsilon_n}, \qquad (3.18)$$

and can set $\bar{\gamma}^2 = 2c'\lambda/\varepsilon_n$.

We recall that the desired theorem in the main paper does not specify the operator A. By linearity we can replace the phrase "for any operator A" in the Theorem by "for any of the n^2 operators $A_{\mu,\nu}$ defined by $(A_{\mu,\nu})_{j,j'} = \delta_{\mu,j}\delta_{\nu,j'}$."

We now let A be one of the $A_{\mu,\nu}$'s, and apply Lemma 1 by setting

$$\Delta = n^2 \|A\|_\infty \left(\frac{\lambda}{\varepsilon_n}\right)^{1/3}, \qquad (3.19)$$

and $\kappa = 1/2$. Then we have

$$\frac{\tau_\Delta(T)}{T} \le \frac{3}{2n^2}\left(\frac{\lambda}{\varepsilon_n}\right)^{-2/3} \bar{\gamma}^2 = \frac{3c'}{n^2}\left(\frac{\lambda}{\varepsilon_n}\right)^{1/3}. \qquad (3.20)$$

Since each of $A_{\mu,\nu}$ can have its own "bad" interval, the total length of the "bad" intervals of all $A_{\mu,\nu}$ is bounded by n^2 times the right-hand side of (3.20). This is what appears in the right-hand side of (15) in the main paper.

It only remains to estimate the systematic difference between the desired $\langle A\rangle_\beta^{\text{can}}$ and $\overline{\langle A\rangle_t}$. We first note that

$$\begin{aligned}
\left| \langle A\rangle^{\text{can}}_{\beta(E')} - \langle A\rangle^{\text{can}}_{\beta(E)} \right| &= \left| \int_E^{E'} dF \frac{d}{dE} \langle A\rangle^{\text{can}}_{\beta(F)} \right| \\
&= \left| \int_E^{E'} dF \frac{d\beta(F)}{dE} \frac{d}{d\beta} \langle A\rangle^{\text{can}}_{\beta(F)} \right| \\
&\le \gamma \left| \int_E^{E'} dF \left(\langle A\varepsilon\rangle^{\text{can}}_{\beta(F)} - \langle A\rangle^{\text{can}}_{\beta(F)} \langle \varepsilon\rangle^{\text{can}}_{\beta(F)} \right) \right| \\
&\le 2\gamma |E' - E| \, \|A\|_\infty \varepsilon_n \\
&\le 2\|A\|_\infty \gamma \left(\lambda + \frac{\varepsilon_n}{2}\right) \varepsilon_n \\
&\le 2\|A\|_\infty \gamma (\varepsilon_n)^2, \qquad (3.21)
\end{aligned}$$

where $\gamma = d\beta(E+\lambda)/dE$. Thus we see

$$\left| \langle A \rangle^{\mathrm{can}}_{\beta(E)} - \sum_{E'} |\gamma_{E'}|^2 \langle A \rangle^{\mathrm{can}}_{\beta(E')} \right| \le 2 \|A\|_\infty \gamma(\varepsilon_n)^2. \tag{3.22}$$

By adding this new systematic error to the error $\sigma \|A\|_\infty$ in the (7) of the main paper, we finally get the statement of the Theorem.

4 Proof of Lemma

In the present rather lengthy section, we shall prove the Lemma in the main paper, which is our main estimate. Throughout the present section, $c_1, c_2, \ldots, c_{23}$ denote positive constants which do not depend on L but may depend on $\{\varepsilon_j\}$, λ, δ, and $\{N_r\}$.

Let us give an outline of the present section. In Section 4.1, we prove the statement of the Lemma, but assuming some new lemmas which will be proved in the latter sections.

In Section 4.2, we introduce the notion of "regular interval", and study how the two index systems ℓ and (j,k) are related with each other. This is essential in getting the desired Boltzmann weights.

In Section 4.3, we decompose the whole region $\{1, 2, \ldots, nN\}$ for the index ℓ into many subintervals.

The next three sections are devoted to the estimate of the solution of the Schrödinger equation (4.1) in each of the above intervals. Therefore the topics of these three sections are asymptotic analyses of a discrete Schrödinger equation, and are not quite specific to the problem of deriving the canonical distribution from quantum dynamics. Although the techniques I use are not quite original, I present all the estimates since I could not find necessary estimates in the literature. In Section 4.4, we treat the solution in the "classically accessible region". The approximate solution is obtained by a speculation based on the quasi-classical analysis, and the difference from the true solution is rigorously controlled by the standard machinery of transfer matrices. In Section 4.5, we treat the solution near the "turning points" where the quasi-classical analysis no longer works. We use the solution of (rescaled) continuous Schrödinger equation as an approximate solution, and control the difference from the true solution inductively. In Section 4.6, we control the solution in the "classically inaccessible regions".

In the next two sections, we extract information about the Boltzmann factor from the controlled approximate solutions of the Schrödinger equation. In Section 4.7, we treat the "classically accessible region". We encounter an annoying phenomenon of "resonance", which locally inhibits the wave function to generate the desired Boltzmann factor. We suspect that this phenomenon is of essential character. In Section 4.8, we get the Boltzmann factor in the region where the wave length of the wave function is long. There are no resonances, and the proof is easy.

In Section 4.9, we fix some exponents, and complete the lengthy proof.

4.1 Proof

We write the Schrödinger equation (4) in the main paper as

$$\varphi_{\ell-1} + \varphi_{\ell+1} + 2\alpha_\ell \varphi_\ell = 0, \tag{4.1}$$

with

$$\alpha_\ell = \frac{U_\ell - E}{\lambda}, \tag{4.2}$$

where E is an eigenvalue such that

$$\varepsilon_n + 2\lambda \le E \le B_{\max} - 2\lambda. \tag{4.3}$$

We shall decompose the whole range of the index ℓ into a disjoint union of Ω intervals as

$$\{1, 2, \ldots, nN\} = \bigcup_{\omega=1}^{\Omega} I_\omega, \tag{4.4}$$

where the intervals I_ω will be specified later in Section 4.3. We here note that I_1 and I_Ω are special intervals which consist of the "classically inaccessible regions" with $\alpha_\ell \le -1$ and $\alpha_\ell \ge 1$, respectively, plus small ranges in the "classically accessible region" attached to them. All the other intervals $I_2, I_3, \ldots, I_{\Omega-1}$ are in the "classically accessible region" $-1 < \alpha_\ell < 1$.

We recall that we have two different index systems, namely, ℓ with $\ell = 1, 2, \ldots, nN$, and (j, k) with $j = 1, 2, \ldots, n$ and $k = 1, 2, \ldots, N$, and these two are in one-to-one correspondence $\ell \leftrightarrow (j, k)$. We make the correspondence manifest by writing

$$\ell \leftrightarrow (j(\ell), k(\ell)), \quad \text{or} \quad \ell(j, k) \leftrightarrow (j, k). \tag{4.5}$$

This is a slight abuse of notation, but we hope there will be no confusions.

The following is our main estimate. It sates that φ_ℓ produces the desired Boltzmann factor in each interval.

Lemma 2 *Let φ_ℓ be a normalized solution of (4.1). For each $\omega = 1, 2, \ldots, \Omega$ and each $j = 1, 2, \ldots, n$, we have*

$$\left| \frac{\sum_{\ell \in I_\omega} \chi[j(\ell) = j] \, |\varphi_\ell|^2}{\sum_{\ell \in I_\omega} |\varphi_\ell|^2} - W_j^{(\omega)} \right| \le c_1 W_j^{(\omega)} L^{-\eta}, \tag{4.6}$$

where the indicator function is defined by $\chi[\text{true}] = 1$ and $\chi[\text{false}] = 0$. The exponent $\eta > 0$ will be determined later in Section 4.9 (to be $1/12$). Here

$$W_j^{(\omega)} = \frac{\rho(U_{\tilde{\ell}(\omega)} - \varepsilon_j)}{\sum_{j'=1}^{n} \rho(U_{\tilde{\ell}(\omega)} - \varepsilon_{j'})} \tag{4.7}$$

is essentially the Boltzmann factor. The index $\tilde{\ell}(\omega)$ are taken from the interval I_ω. For the intervals I_1 and I_Ω, we take the corresponding $\tilde{\ell}(1)$ and $\tilde{\ell}(\Omega)$ from the "classically accessible parts" of the intervals.

This lemma will be proved in subsequent sections by constructing local approximations for φ_ℓ.

Given this lemma,we immediately get

Lemma 3 *Let φ_ℓ be a normalized solution of (4.1). For each $j = 1, 2, \ldots, n$, we have*

$$\left| \sum_{k=1}^{N} \left| \varphi_{(j,k)} \right|^2 - W_j \right| \le c_1 W_j L^{-\eta}, \tag{4.8}$$

with W_j satisfying

$$\sum_{j=1}^{n} W_j = 1, \tag{4.9}$$

and

$$\frac{\rho(E - \varepsilon_j - \lambda)}{\sum_{j'=1}^{n} \rho(E - \varepsilon_{j'} + \lambda)} \le W_j \le \frac{\rho(E - \varepsilon_j + \lambda)}{\sum_{j'=1}^{n} \rho(E - \varepsilon_{j'} - \lambda)}. \tag{4.10}$$

Proof: This is almost trivial. By writing $P_\omega = \sum_{\ell \in I_\omega} |\varphi_\ell|^2$, we have

$$\begin{aligned} \sum_{k=1}^{N} \left| \varphi_{(j,k)} \right|^2 &= \sum_{\ell=1}^{nN} \chi[j(\ell) = j] |\varphi_\ell|^2 \\ &= \sum_{\omega=1}^{\Omega} P_\omega \frac{\sum_{\ell \in I_\omega} \chi[j(\ell) = j] |\varphi_\ell|^2}{\sum_{\ell \in I_\omega} |\varphi_\ell|^2}. \end{aligned} \tag{4.11}$$

Since we have $\sum_{\omega=1}^{\Omega} P_\omega = 1$ and $P_\omega \ge 0$, (4.6) immediately implies (4.8) with

$$W_j = \sum_{\omega=1}^{\Omega} P_\omega W_j^{(\omega)}. \tag{4.12}$$

The normalization property (4.9) is trivial if we note (4.7) and (4.12). The bound (4.10) follows from (4.7) and (4.12) if we note $E - \lambda \le U_{\tilde{\ell}(\omega)} \le E + \lambda$ for $\omega = 1, 2, \ldots, \Omega$ and ρ is nondecreasing. ■

For any operator A on the Hilbert space $\mathcal{H}_{\mathrm{S}}$ of the subsystem (with the matrix elements $(A)_{j,j'} = \langle \Psi_j, A \Psi_{j'} \rangle$), we define

$$\langle A \rangle_W = \sum_{j=1}^{n} (A)_{j,j} W_j. \tag{4.13}$$

We show that this expectation value is almost equal to the desired canonical expectation value

$$\langle A \rangle_\beta^{\mathrm{can}} = \frac{\mathrm{Tr}_{\mathrm{S}}[A e^{-\beta H_{\mathrm{S}}}]}{\mathrm{Tr}_{\mathrm{S}}[e^{-\beta H_{\mathrm{S}}}]} = \frac{\sum_{j=1}^{n} (A)_{j,j} e^{-\beta \varepsilon_j}}{\sum_{j=1}^{n} e^{-\beta \varepsilon_j}}. \tag{4.14}$$

This is an elementary estimate, and can be proved rather easily.

Lemma 4 *For any operator A on $\mathcal{H}_{\mathrm{S}}$, we have*

$$\left|\langle A\rangle_W - \langle A\rangle_\beta^{\mathrm{can}}\right| \|A\|_\infty \left\{3\beta\gamma + \gamma(\varepsilon_n)^2\right\}, \tag{4.15}$$

with $\beta = \beta(E) = d\log\rho(E)/dE$ and $\gamma = d\beta(E+\lambda)/dE$.

Proof: Let $\widetilde{E}_j = E - \varepsilon_j$. We shall prove upper and lower bounds for $\rho(\widetilde{E}_j \pm \lambda)/\rho(\widetilde{E}_1)$. Since $\beta(E) = d\log\rho(E)/dE$, we have

$$\frac{\rho(\widetilde{E})}{\rho(\widetilde{E}_1)} = \exp\left[\int_{\widetilde{E}_1}^{\widetilde{E}} dE\,\beta(E)\right], \tag{4.16}$$

for any $\widetilde{E}$. By expanding $\beta(\widetilde{E})$ around $\widetilde{E}_1$ and recalling that $d\beta(E)/dE$ is increasing, we have

$$0 \le \int_{\widetilde{E}_1}^{\widetilde{E}} \beta(E) - (\widetilde{E}-\widetilde{E}_1)\beta(\widetilde{E}_1) \le \frac{\gamma}{2}(\widetilde{E}-\widetilde{E}_1)^2, \tag{4.17}$$

where $\gamma = \beta'(\widetilde{E}_1+\lambda)$. Substituting these bounds into (4.16), we have

$$\begin{aligned}\frac{\rho(\widetilde{E}_j+\lambda)}{\rho(\widetilde{E}_1)} &\le e^{-\beta(\varepsilon_j-\varepsilon_1)+\beta\lambda+(\gamma/2)(\varepsilon_j-\varepsilon_1-\lambda)^2} \\ &\le e^{-\beta(\varepsilon_j-\varepsilon_1)+\beta\lambda+(\gamma/2)(\varepsilon_n-\varepsilon_1)^2},\end{aligned} \tag{4.18}$$

and

$$\frac{\rho(\widetilde{E}_j-\lambda)}{\rho(\widetilde{E}_1)} \ge e^{-\beta(\varepsilon_j-\varepsilon_1)-\beta\lambda}, \tag{4.19}$$

with $\beta = \beta(\widetilde{E}_1)$ for any $j = 1, 2, \ldots, n$. By substituting (4.18), (4.19) into (4.10), we finally get

$$e^{-2\beta\lambda-(\gamma/2)(\varepsilon_n-\varepsilon_1)^2} \le \frac{W_j}{\widetilde{W}_j^{(\beta)}} \le e^{2\beta\lambda+(\gamma/2)(\varepsilon_n-\varepsilon_1)^2}, \tag{4.20}$$

where $\widetilde{W}_j^{(\beta)} = e^{-\beta\varepsilon_j}/\sum_{j'=1}^n e^{-\beta\varepsilon_{j'}}$ is the Boltzmann factor.

We can finish the proof of (4.15) by observing that

$$\begin{aligned}\left|\langle A\rangle_W - \langle A\rangle_\beta^{\mathrm{can}}\right| &= \left|\sum_{j=1}^n (A)_{j,j}(W_j - \widetilde{W}_j^{(\beta)})\right| \\ &\le \left\{\sum_{j=1}^n |(A)_{j,j}|\,\widetilde{W}_j^{(\beta)}\right\}\max_j\left|\frac{W_j}{\widetilde{W}_j^{(\beta)}} - 1\right| \\ &\le \|A\|_\infty\left\{3\beta\lambda + \gamma(\varepsilon_n-\varepsilon_1)^2\right\},\end{aligned} \tag{4.21}$$

where the final line follows form (4.20) if $2\beta\lambda + (\gamma/2)(\varepsilon_n-\varepsilon_1)^2 \le 0.7$, which we shall assume. ■

To complete the proof of the Lemma in the main paper, we need one more estimate which will be proved in Section 4.6.

Lemma 5 *For any normalized φ_ℓ satisfying (4.1), we have*

$$\sum_{k=1}^{N} \overline{\varphi_{(j,k)}}\varphi_{(j',k)} \le \text{const.}e^{-\text{const.}L^{1/3}}, \tag{4.22}$$

for any $j \neq j'$.

Given all the above estimates, to prove the desired Lemma in the main paper is straightforward. With the expansion

$$\Phi_E = \sum_{j=1}^{n}\sum_{k=1}^{N} \varphi_{(j,k)}\,\Psi_j \otimes \Gamma_k, \tag{4.23}$$

the desired quantity becomes

$$\langle \Phi_E, (A \otimes \mathbf{1}_\mathrm{B})\Phi_E\rangle = \sum_{j,j'=1}^{n} (A)_{j,j'} \left\{ \sum_{k=1}^{N} \overline{\varphi_{(j,k)}}\varphi_{(j',k)} \right\}. \tag{4.24}$$

Since the diagonal weigh $\sum_{k=1}^{N} |\varphi_{(j,k)}|^2$ is controlled by (4.8), and the off diagonal weight $\sum_{k=1}^{N} \overline{\varphi_{(j,k)}}\varphi_{(j',k)}$ for $j \neq j'$ by (4.22), we immediately see that

$$|\langle \Phi_E, (A \otimes \mathbf{1}_\mathrm{B})\Phi_E\rangle - \langle A\rangle_W| \le 2c_1 \|A\|_\infty L^{-\eta}. \tag{4.25}$$

By combining this with the systematic error estimate (4.15), we get the desired (7) of the main paper.

4.2 Regular intervals

We first recall special regular structure of the spectrum $\{B_k\}_{k=1,\dots,N}$ of H_B. In each interval $((r-1)\delta, r\delta)$ with $r = 1, 2, \dots, R$, the energy eigenvalues B_k are spaced with exactly equal spacing $b_r = \delta(M_r L)^{-1}$. This means that the whole index set is naturally decomposed into R intervals as $\{1, 2, \dots, N\} = \bigcup_{r=1}^{R} K_R$, so that for any $k \in K_r$, we have $B_k \in ((r-1)\delta, r\delta)$.

Since $U_{(j,k)} = \varepsilon_j + B_k$, the structure of $\{U_\ell\}$ inherits the above regularity of $\{B_k\}$. We say that an interval $J \subset \{1, 2, \dots, nN\}$ is *regular* if for any $(j,k) \leftrightarrow \ell \in J$, we have $k \in K_{r(j)}$ with (J-dependent) $r(1), r(2), \dots, r(n)(= 1, 2, \dots, R)$. Thus, in the interval J, U_ℓ is constructed by superposing n shifted copies of $\{B_k\}$ each of them having exactly equal level spacings.

The whole range of ℓ can be decomposed into a disjoint union as

$$\{1, 2, \dots, nN\} = \bigcup_{s=1}^{nR} J_s, \tag{4.26}$$

where each J_s is a maximal regular interval. We note that each regular interval has length of $O(L)$. We also remark that (4.26) is not yet the decomposition (4.4).

We want to determine the behavior of the index $\ell(j,k)$, U_ℓ, and $\alpha_\ell = (U_\ell - E)/\lambda$ in a fixed regular interval J, which is one of $J_1, \dots, J_{nR}$. For simplicity, we write

$$\tilde{b}_j = b_{r(j)}, \quad \widetilde{M}_j = M_{r(j)}, \tag{4.27}$$

for $j = 1, 2, \ldots, n$.

Let $(j,k) \leftrightarrow \ell \in J$. Because of the regularity, we can write

$$U_{(j,k)} = (k - \kappa_j)\tilde{b}_j + u_j, \tag{4.28}$$

for some κ_j and u_j (which are again J-dependent). The index ℓ is determined by ordering $U_{(j,k)}$ so that $U_\ell \leq U_{\ell+1}$.

To get an explicit formula for $\ell(j,k)$, we count the number of $(j',k') \in J$ such that

$$U_{(j',k')} \leq U_{(j,k)}. \tag{4.29}$$

For a fixed $j' \neq j$, the number of k' with (4.29) is

$$\left[\frac{U_{(j,k)} - u_{j'}}{\tilde{b}_{j'}} \right], \tag{4.30}$$

where $[\cdots]$ is the Gauss symbol. Summing up these contribution as well as that from the indexes $(j,k') \in J$, we get

$$\begin{aligned} \ell(j,k) &= \ell_0 - 1 + (k - \kappa_j) + 1 + \sum_{j' \neq j} \left[\frac{U_{(j,k)} - u_{j'}}{\tilde{b}_{j'}} \right] \\ &= \ell_0 + \sum_{j'=1}^{n} \left[\frac{(k - \kappa_j)\tilde{b}_j + u_j - u_{j'}}{\tilde{b}_{j'}} \right], \end{aligned} \tag{4.31}$$

where we used (4.28), and ℓ_0 is the smallest index in J. For the latter use, we substitute the relation $\tilde{b}_j = \delta(\widetilde{M}_j L)^{-1}$ into (4.31) to get

$$\ell(j,k) = \ell_0' + \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j} k + \eta_{j.j'} \right], \tag{4.32}$$

where ℓ_0' and $\eta_{j,j'}$ are constants (which may depend on L).

From (4.31), we see that

$$\tilde{\ell}(j,k) - (n-1) \leq \ell(j,k) \leq \tilde{\ell}(j,k), \tag{4.33}$$

with

$$\tilde{\ell}(j,k) = \ell_0 + \sum_{j'=1}^{n} \frac{(k - \kappa_j)\tilde{b}_j + u_j - u_{j'}}{\tilde{b}_{j'}}. \tag{4.34}$$

Let

$$\bar{b} = \left(\sum_{j=1}^{n} \frac{1}{\tilde{b}_j} \right)^{-1}. \tag{4.35}$$

Note that

$$\bar{b} = \left(\sum_{j=1}^{n} \frac{\widetilde{M}_j L}{\delta} \right)^{-1} = \left(\frac{\delta}{\sum_{j=1}^{n} \widetilde{M}_j} \right) L^{-1} = \frac{g\lambda}{L}, \tag{4.36}$$

where

$$g = \frac{\delta}{\lambda \sum_{j=1}^{n} \widetilde{M}_j} \tag{4.37}$$

is an L-independent quantity. Observe that

$$\begin{aligned} \bar{b}\left\{\tilde{\ell}(j,k) - \ell_0\right\} &= (k-\kappa_j)\tilde{b}_j + u_j - \bar{u} \\ &= U_{(j,k)} - \bar{u}, \end{aligned} \tag{4.38}$$

where

$$\bar{u} = \bar{b}\sum_{j=1}^{n} \frac{u_j}{\tilde{b}_j} \tag{4.39}$$

is an energy near the bottom of the interval J. From (4.38) and (4.33), we get

$$\bar{b}\ell + \widetilde{U} \le U_\ell \le \bar{b}\ell + \widetilde{U} + \bar{b}(n-1), \tag{4.40}$$

for ℓ in the regular interval J, where $\widetilde{U} = \bar{u} - \bar{b}\ell_0$.

We introduce a linearized α_ℓ by

$$\overline{\alpha}_\ell = \frac{\bar{b}\ell + \widetilde{U} - E}{\lambda} = g\frac{\ell}{L} + \frac{\widetilde{U} - E}{\lambda}, \tag{4.41}$$

for $\ell \in J$. Then from (4.40), we find

$$|\alpha_\ell - \overline{\alpha}_\ell| \le \frac{\bar{b}(n-1)}{\lambda} = \frac{g(n-1)}{L}. \tag{4.42}$$

4.3 Decomposition into intervals

We describe precise definitions of the decomposition (4.4) of the intervals. The intervals $I_1, \ldots, I_\Omega$ are properly ordered, and covers the whole range $\{1, 2, \ldots, nN\}$ without any overlaps.

We define the first turning point ℓ_{t} as the minimum ℓ such that $\alpha_\ell > -1$. Then the first interval is defined as

$$I_1 = \left\{1, 2, \ldots, \ell_{\mathrm{t}} + [c_2 L^{1/3}]\right\}. \tag{4.43}$$

Again $[\cdots]$ is the Gauss symbol. Similarly we define

$$I_\Omega = \left\{\ell'_{\mathrm{t}} - [c_2 L^{1/3}], \ldots, nN\right\}, \tag{4.44}$$

where the second turning point ℓ'_{t} is the maximum ℓ such that $\alpha_\ell < 1$.

The intervals $I_2, \ldots, I_\Gamma$ all have the length $|I_\omega| = [c_3 L^{(1/3)-\eta}]$. Γ is determined as the minimum number such that $\sum_{\omega=2}^{\Gamma} |I_\omega| \ge [c_4 L^{1-\varepsilon}]$. The exponent $\varepsilon > 0$ will be determined later, but it must satisfy

$$1 - \varepsilon > \frac{1}{3} - \eta, \tag{4.45}$$

because we must have $\sum_{\omega'=2}^{\Gamma} |I_{\omega'}| \ge |I_\omega|$. Similarly the intervals $I_{\Omega-\Gamma+1}, \ldots, I_{\Omega-1}$ have the length $[c_3 L^{(1/3)-\eta}]$.

The remaining intervals $I_{\Gamma+1}, \ldots, I_{\Omega-\Gamma}$ are defined to cover the (wide) remaining region $\Big\{\ell_{\mathrm{t}} + [c_2 L^{1/3}] + [c_4 L^{1-\varepsilon}], \ldots, \ell_{\mathrm{t}} - [c_2 L^{1/3}] - [c_4 L^{1-\varepsilon}]\Big\}$. We require for $\omega = \Gamma+1, \ldots, \Omega-\Gamma$ that I_ω has the length

$$[c_5 L^{1-2\theta}/2] \le |I_\omega| \le [c_5 L^{1-2\theta}], \tag{4.46}$$

where θ is an exponent to be determined later, and I_ω is contained in a single regular interval defined in Section 4.2. These two conditions are easily satisfied since the lengths of the regular intervals are of $O(L)$.

4.4 Approximate solutions in the "classically accessible region"

We will construct approximate solutions of the Schrödinger equation (4.1) in the intervals $I_2, \ldots, I_{\Omega-1}$, which are within the "classically accessible region".

For simplicity, we denote by $I = \{\ell_1, \ell_1+1, \cdots, \ell_2\}$ one of the intervals $I_2, \ldots, I_{\Omega-1}$. Since the interval I is entirely contained in a single regular interval J, we have corresponding $\overline{\alpha}_\ell$ defined by (4.41), which is a linear approximation to α_ℓ. We also write

$$\alpha = \alpha_{\ell_2}, \quad \beta = \alpha_{\ell_1}. \tag{4.47}$$

We start from an abstract theory for (rigorously) evaluating the difference between an approximate solution and the true solution of (4.1). Let ψ_ℓ be an approximate solution of (4.1) with α_ℓ replaced by its linearlization $\overline{\alpha}_\ell$ in the sense that

$$\psi_{\ell+1} + \psi_{\ell-1} + 2\overline{\alpha}_\ell \psi_\ell = \delta_\ell \tag{4.48}$$

holds for $\ell \in \bar{I} = \{\ell_1+1, \ldots, \ell_2-1\}$. Here δ_ℓ is an error term, which must be small.

For a solution φ_ℓ of the original Schrödinger equation (4.1), we write the deviation from the approximate solution as

$$f_\ell = \varphi_\ell - \psi_\ell. \tag{4.49}$$

From (4.1) and (4.48), we find

$$f_{\ell+1} + f_{\ell-1} + 2\alpha_\ell f_\ell = \sigma_\ell, \tag{4.50}$$

with

$$\sigma_\ell = 2(\overline{\alpha}_\ell - \alpha_\ell)\psi_\ell - \delta_\ell. \tag{4.51}$$

As usual the equation (4.50) can be written in a matrix form as

$$\begin{pmatrix} f_{\ell+1} \\ f_\ell \end{pmatrix} = \mathsf{T}_\ell \begin{pmatrix} f_\ell \\ f_{\ell-1} \end{pmatrix} + \begin{pmatrix} \sigma_\ell \\ 0 \end{pmatrix}, \tag{4.52}$$

where the transfer matrix is

$$\mathsf{T}_\ell = \begin{pmatrix} -2\alpha_\ell & -1 \\ 1 & 0 \end{pmatrix}. \tag{4.53}$$

Considering the second order nature of the equations (4.1) and (4.48), we can assume without loosing generality that $f_{\ell_1} = f_{\ell_1+1} = 0$. Then by inserting (4.52), we find

$$\begin{pmatrix} f_{\ell+1} \\ f_\ell \end{pmatrix} = \sum_{k=\ell_1+1}^{\ell} \mathsf{T}_\ell \mathsf{T}_{\ell-1} \cdots \mathsf{T}_{k+1} \begin{pmatrix} \sigma_k \\ 0 \end{pmatrix}. \tag{4.54}$$

Since we have $|\alpha_\ell| < 1$ in the "classically accessible region", the transfer matrix T_ℓ of (4.53) has two eigenvalues $e_\ell, \overline{e_\ell}$ with $|e_\ell| = |\overline{e_\ell}| = 1$, where

$$e_\ell = -\alpha_\ell + i\sqrt{1-{\alpha_\ell}^2}. \tag{4.55}$$

Thus there exists a regular matrix M_ℓ such that

$$(\mathsf{M}_\ell)^{-1}\mathsf{T}_\ell\mathsf{M}_\ell = \begin{pmatrix} e_\ell & 0 \\ 0 & \overline{e_\ell} \end{pmatrix}. \tag{4.56}$$

Let us define

$$\mathsf{D}_\ell = (\mathsf{M}_\ell)^{-1}\mathsf{M}_{\ell-1} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.57}$$

which is expected to be small since M_ℓ and $\mathsf{M}_{\ell-1}$ are very similar with each other. Then from (4.56), we have

$$\begin{aligned}
&\mathsf{T}_\ell\mathsf{T}_{\ell-1}\cdots\mathsf{T}_{k+1} \\
&= \mathsf{M}_\ell \begin{pmatrix} e_\ell & 0 \\ 0 & \overline{e_\ell} \end{pmatrix} (\mathsf{M}_\ell)^{-1}\mathsf{M}_{\ell-1} \begin{pmatrix} e_{\ell-1} & 0 \\ 0 & \overline{e_{\ell-1}} \end{pmatrix} (\mathsf{M}_{\ell-1})^{-1}\cdots \\
&\cdots\mathsf{M}_{k+1} \begin{pmatrix} e_{k+1} & 0 \\ 0 & \overline{e_{k+1}} \end{pmatrix} (\mathsf{M}_{k+1})^{-1} \\
&= \mathsf{M}_\ell \begin{pmatrix} e_\ell & 0 \\ 0 & \overline{e_\ell} \end{pmatrix} (\mathbf{1}+\mathsf{D}_\ell) \begin{pmatrix} e_{\ell-1} & 0 \\ 0 & \overline{e_{\ell-1}} \end{pmatrix} (\mathbf{1}+\mathsf{D}_{\ell-1})\cdots \\
&\cdots(\mathbf{1}+\mathsf{D}_{k+2}) \begin{pmatrix} e_{k+1} & 0 \\ 0 & \overline{e_{k+1}} \end{pmatrix} (\mathsf{M}_{k+1})^{-1}.
\end{aligned} \tag{4.58}$$

For any $a, b = 1, 2$, we denote by $(\mathsf{A})_{a,b}$ the a,b-component of a 2×2 matrix A. We now assume that

$$|(\mathsf{D}_\ell)_{a,b}| \le d_\ell, \tag{4.59}$$

for any $a, b = 1, 2$. Then (4.58) implies

$$\begin{aligned}
|(\mathsf{T}_\ell\mathsf{T}_{\ell-1}\cdots\mathsf{T}_{k+1})_{a,b}| &\le \|\mathsf{M}_\ell\|_\infty \left\|(\mathsf{M}_{k+1})^{-1}\right\|_\infty \prod_{j=k+1}^{\ell}(1+2d_j) \\
&\le \|\mathsf{M}_\ell\|_\infty \left\|(\mathsf{M}_{k+1})^{-1}\right\|_\infty \exp\left[2\sum_{j=k+1}^{\ell} d_j\right].
\end{aligned} \tag{4.60}$$

To make the estimate (4.60) more concrete, we fix precise form of M_ℓ as

$$\mathsf{M}_\ell = \frac{1}{\sqrt{2}(1-{\alpha_\ell}^2)^{1/4}} \begin{pmatrix} e_\ell & \overline{e_\ell} \\ 1 & 1 \end{pmatrix}, \tag{4.61}$$

whose inverse is

$$(\mathsf{M}_\ell)^{-1} = \frac{1}{i\sqrt{2}(1-{\alpha_\ell}^2)^{1/4}} \begin{pmatrix} 1 & -\overline{e_\ell} \\ -1 & e_\ell \end{pmatrix}. \tag{4.62}$$

Since D_ℓ defined by (4.57) is vanishing if $\alpha_\ell = \alpha_{\ell-1}$, we can evaluate D_ℓ by expanding it in $(\alpha_\ell - \alpha_{\ell-1})$. Then we find that essential contribution comes from the first order in the expansion, and the desired bound (4.59) is satisfied with

$$d_\ell = \frac{\alpha_\ell - \alpha_{\ell-1}}{1 - {\alpha_\ell}^2}, \tag{4.63}$$

provided that

$$1 - {\alpha_\ell}^2 \geq \frac{2}{L}, \tag{4.64}$$

which is automatically satisfied in the present interval. Substituting (4.63) into (4.60), we find

$$|(\mathsf{T}_\ell \mathsf{T}_{\ell-1} \cdots \mathsf{T}_{k+1})_{a,b}| \leq \|\mathsf{M}_\ell\|_\infty \left\|(\mathsf{M}_{k+1})^{-1}\right\|_\infty \exp\left[\frac{2(\alpha_\ell - \alpha_{k+1})}{1-\gamma^2}\right], \tag{4.65}$$

for any $a, b = 1, 2$, where γ is one of α_ℓ with $\ell \in I$ which gives the smallest $1 - {\alpha_\ell}^2$.

At this stage, we impose a condition on I that

$$\frac{\alpha - \beta}{1 - \gamma^2} \leq c_6, \tag{4.66}$$

where α, β are defined by (4.47). Then (4.65) simplifies as

$$\begin{aligned} |(\mathsf{T}_\ell \mathsf{T}_{\ell-1} \cdots \mathsf{T}_{k+1})_{a,b}| &\leq \|\mathsf{M}_\ell\|_\infty \left\|(\mathsf{M}_{k+1})^{-1}\right\|_\infty e^{c_6} \\ &\leq c_7 (1 - {\alpha_\ell}^2)^{-1/4} (1 - {\alpha_k}^2)^{-1/4}, \end{aligned} \tag{4.67}$$

where we used (4.61) and (4.62). Substituting (4.67) to (4.54), we get a useful bound

$$|f_{\ell+1}| \leq \frac{c_7}{(1-{\alpha_\ell}^2)^{1/4}(1-\gamma^2)^{1/4}} \sum_{k=\ell_1+1}^{\ell} |\sigma_k|. \tag{4.68}$$

This completes the general theory.

We now explicitly construct an approximate solution ψ_ℓ which appears in (4.48). We first define ζ_ℓ by

$$\cos \zeta_\ell = -\overline{\alpha}_\ell. \tag{4.69}$$

Since $\overline{\alpha}_\ell$ is increasing in ℓ and satisfies $|\overline{\alpha}_\ell| < 1$, we see that ζ_ℓ is increasing and satisfies $0 < \zeta_\ell < \pi$. Let us define

$$Z_\ell = \left(\sum_{\ell'=\ell_1}^{\ell-1} \zeta_{\ell'} \right) + \frac{\zeta_\ell}{2}. \tag{4.70}$$

Then we can write down our approximate solution as

$$\psi_\ell = \frac{\cos(Z_\ell + \xi)}{\sqrt{\sin \zeta_\ell}}, \tag{4.71}$$

where ξ is an arbitrary constant. The form (4.71) is (heuristically) obtained by following the standard idea of quasi-classical analysis. We learned that this approximate solution was written down long time ago by Bethe[2].

[2] H. Bethe, Phys. Rev. **54**, 955 (1938).

We now need an estimate for the error term δ_ℓ which appears in (4.48). To do this, we substitute the concrete form (4.71) into the left-hand side of (4.48), and expand the resulting quantity in a power series of $(\overline{\alpha}_{\ell+1}-\overline{\alpha}_\ell)=(\overline{\alpha}_\ell-\overline{\alpha}_{\ell-1})=\bar{b}/\lambda(=g/L)$. (See (4.41.) We find that the first order terms cancel out, and the essential contribution comes from the second order. We skip the tedious but straightforward calculation, and describe only the final result, which is

$$\begin{aligned}|\delta_\ell| &\le \frac{1}{2(1-(\overline{\alpha}_\ell)^2)^{3/4}}\frac{\alpha_\ell}{(1-(\overline{\alpha}_\ell)^2)^{3/2}}\left(\frac{\bar{b}}{\lambda}\right)^2\\ &\quad+\frac{2}{(1-(\overline{\alpha}_\ell)^2)^{5/4}}\left(\frac{\bar{b}}{\lambda(1-(\overline{\alpha}_\ell)^2)^{1/2}}\right)^2\\ &\le \frac{3}{(1-(\overline{\alpha}_\ell)^2)^{9/4}}\left(\frac{\bar{b}}{\lambda}\right)^2.\end{aligned}\tag{4.72}$$

Here we used the fact that $\alpha_\ell\simeq\overline{\alpha}_\ell$ in the sense of (4.42).

By recalling the definition (4.51) of σ_ℓ, and using (4.72) and (4.42), we find

$$|\sigma_\ell|\le\frac{2n}{(1-{\alpha_\ell}^2)^{1/4}}\left(\frac{\bar{b}}{\lambda}\right)+\frac{3}{(1-{\alpha_\ell}^2)^{9/4}}\left(\frac{\bar{b}}{\lambda}\right)^2,\tag{4.73}$$

where we noted that $\sin\zeta_\ell=\sqrt{1-{\alpha_\ell}^2}$. Since

$$\sum_{k=\ell_1+1}^{\ell}\frac{\bar{b}}{\lambda}=\overline{\alpha}_\ell-\overline{\alpha}_{\ell_1}\simeq\alpha_\ell-\alpha_{\ell_1},\tag{4.74}$$

we find

$$\sum_{k=\ell_1+1}^{\ell}|\sigma_k|\le\frac{2n(\alpha-\beta)}{(1-\gamma^2)^{1/4}}+\frac{3(\alpha-\beta)}{(1-\gamma^2)^{9/4}}\left(\frac{\bar{b}}{\lambda}\right).\tag{4.75}$$

Going back to (4.68), we finally see that the relative error is bounded as

$$\begin{aligned}\left|f_\ell\sqrt{\sin\zeta_\ell}\right| &\le \frac{c_7}{(1-\gamma^2)^{1/4}}\sum_{k=\ell_1+1}^{\ell}|\sigma_k|\\ &\le \frac{2nc_7(\alpha-\beta)}{(1-\gamma^2)^{1/2}}+\frac{3c_7(\alpha-\beta)}{(1-\gamma^2)^{5/2}}\left(\frac{\bar{b}}{\lambda}\right).\end{aligned}\tag{4.76}$$

For the latter uses, we want to get a bound of the form

$$\left|f_\ell\sqrt{\sin\zeta_\ell}\right|\le c_8L^{-\eta},\tag{4.77}$$

with a constant c_8 which does not depend on L and the specific interval.

We shall write down conditions that the exponents η, ε and θ should satisfy to get (4.77). We start from the case where I is one of the second type intervals, i.e., I_ω with $\omega=2,\ldots,\Gamma$ or $\omega=\Omega-\Gamma+1,\ldots,\Omega-1$. These are the intervals which are relatively close to the turning points. For such an interval, we have $1-\gamma^2\ge c_2L^{1/3}(\bar{b}/\lambda)=c_2gL^{-2/3}$.

(See (4.37) for the definition of g, which is an L-independent quantity.) We also find $(\alpha-\beta) \le c_3 L^{(1/3)-\eta}(\bar{b}/\lambda) = c_3 g L^{-(2/3)-\eta}$. It is easy to check that the condition (4.66) is satisfied. By substituting these bound into (4.76), we see that

$$\left| f_\ell \sqrt{\sin \zeta_\ell} \right| \le 2nc_7c_3\sqrt{\frac{g}{c_2}} L^{-(1/3)-\eta} + \frac{3c_7c_3}{\sqrt{{c_2}^5 g}} L^{-\eta}. \tag{4.78}$$

Thus we find that the desired bound (4.77) is indeed satisfied.

We then consider the case where I is one of the third type intervals, i.e., I_ω with $\omega = \Gamma+1,\ldots,\Omega-\Gamma$. Here we have $(1-\gamma^2) \ge c_4 L^{1-\varepsilon}(\bar{b}/\lambda) = c_4 g L^{-\varepsilon}$, and $(\alpha-\beta) \le c_5 L^{1-2\theta}(\bar{b}/\lambda) = c_5 g L^{-2\theta}$. Therefore the condition (4.66) is satisfied if

$$-2\theta + \varepsilon \le 0. \tag{4.79}$$

Substituting these bounds into (4.76), we get

$$\begin{aligned} \left| f_\ell \sqrt{\sin \zeta_\ell} \right| &\le 2nc_7c_5\sqrt{\frac{g}{c_4}} L^{-2\theta+(\varepsilon/2)} + \frac{3c_7c_5}{\sqrt{{c_4}^5 g}} L^{-1-2\theta+(5\varepsilon/2)}. \\ &= \left(2nc_7c_5\sqrt{\frac{g}{c_4}} + \frac{3c_7c_5}{\sqrt{{c_4}^5 g}} L^{2\varepsilon-1} \right) L^{-2\theta+(\varepsilon/2)}. \end{aligned} \tag{4.80}$$

Therefore, we have the desired bound (4.76) provided that

$$\varepsilon \le \frac{1}{2}, \tag{4.81}$$

and

$$-2\theta + \frac{\varepsilon}{2} \le -\eta. \tag{4.82}$$

Later in Section 4.9, we determine all the exponents appear in the proof. As these exponents, we will set $\eta = \theta = 1/6$ and $\varepsilon = 1/3$, which satisfy (4.81) and (4.82).

To summarize, we have proved

Lemma 6 *Let φ_ℓ be a real solution of (4.1). Let I be one of the intervals I_ω with $\omega = 2,\ldots,\Omega-1$. There are real constants A and ξ, and we have*

$$\left| \varphi_\ell - A\frac{\cos(Z_\ell+\xi)}{\sqrt{\sin\zeta_\ell}} \right| \le c_8 \frac{A}{\sqrt{\sin\zeta_\ell}} L^{-\eta}, \tag{4.83}$$

for $\ell \in I$.

4.5 Approximate solutions near the "turning points"

We will construct approximate solutions of the Schrödinger equation (4.1) in the "classically accessible parts" of the intervals I_1 and I_Ω. The remaining "classically inaccessible parts" will be discussed in Section 4.6. Near the turning points, the wave length of the oscillation of φ_ℓ becomes long and the quasi-classical approximation becomes useless. Instead we try to approximate φ_ℓ by the solution of a rescaled continuous Schrödinger equation that corresponds to (4.1).

Let us discuss the interval I_1 which contains the first turning point ℓ_{t} at which $\alpha_{\ell_{\mathrm{t}}} \simeq 1$. The treatment of I_Ω is essentially the same. We want to construct approximate solution of φ_ℓ for ℓ in the interval $\tilde{I}_1 = \left\{\ell_{\mathrm{t}}, \ell_{\mathrm{t}}+1, \ldots, \ell_{\mathrm{t}}+[c_2 L^{1/3}]\right\} \subset I_1$. let us write

$$\beta_\ell = 2(\alpha_\ell + 1), \tag{4.84}$$

and rewrite the Schrödinger equation (4.1) as

$$\varphi_{\ell-1} - 2\varphi_\ell + \varphi_{\ell+1} + \beta_\ell \varphi_\ell = 0. \tag{4.85}$$

From (4.41) and (4.42), we find that

$$\left|\beta_\ell - \left(\frac{\bar{b}}{\lambda}\right)(\ell - \ell_{\mathrm{t}})\right| \le \frac{2(n-1)\bar{b}}{\lambda} = 2(n-1)gL^{-1}. \tag{4.86}$$

We want to approximate φ_ℓ by a continuous function $\psi(x)$ with $x = L^{-1/3}(\ell - \ell_{\mathrm{t}})$. With this correspondence in mind, we divide (4.85) by $(L^{-1/3})^2$ to (roughly) get

$$\psi''(x) + L^{-2/3}\beta_\ell \psi(x) \simeq 0. \tag{4.87}$$

We then note that

$$L^{-2/3}\beta_\ell \simeq L^{-2/3}\frac{g}{L}(\ell - \ell_{\mathrm{t}}) = gx. \tag{4.88}$$

So we are motivated to consider the continuous Schrödinger equation

$$\psi''(x) + gx\,\psi(x) = 0. \tag{4.89}$$

Let $\psi(x)$ be the solution of (4.89) in the region $x \ge 0$. By an explicit calculation, one finds that two independent complex solutions of (4.89) are given by

$$\psi(x) = \sqrt{x}\,h[(2/3)\sqrt{g}x^{3/2}], \tag{4.90}$$

and $\overline{\psi(x)}$, where

$$h(z) = H^{(1)}_{1/3}(z) = J_{1/3}(z) + iY_{1/3}(z) \tag{4.91}$$

is the Hankel function (or Bessel's function of the third kind). From the asymptotic behavior of the Hankel function, we find

$$\psi(x) \approx x^{-1/4}\exp\left[i\left\{(2/3)\sqrt{g}x^{3/2} - (5\pi/12)\right\}\right], \tag{4.92}$$

for $x \gg 1$.

From now on, we use the index $m = \ell - \ell_{\mathrm{t}}$ for convenience. To control the approximation rigorously, we first Taylor expand $\psi(L^{-1/3}(m \pm 1))$ to get

$$\psi(L^{-1/3}(m+1)) - 2\psi(L^{-1/3}m) + \psi(L^{-1/3}(m-1)) = L^{-2/3}\psi''(L^{-1/3}m) + L^{-1}\nu_m, \tag{4.93}$$

where

$$\nu_m = \frac{1}{6}\{\psi'''(x') + \psi'''(x'')\} \simeq \frac{1}{3}\psi'''(L^{-1/3}m), \tag{4.94}$$

with $L^{-1/3}(m+1) \le x' \le L^{-1/3}m \le x'' \le L^{-1/3}(m-1)$. By using (4.89) and (4.93), we find

$$\psi(L^{-1/3}(m+1)) - 2\psi(L^{-1/3}m) + \psi(L^{-1/3}(m-1)) = -\frac{\bar{b}}{\lambda}m\psi(L^{-1/3}m) + L^{-1}\nu_m, \quad (4.95)$$

where we noted that $L^{-2/3}gL^{-1/3}m = (\bar{b}/\lambda)m$. We divide the equation (4.95) by $\psi(L^{-1/3}(m+1))$ to get

$$\begin{aligned} &1 - 2\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))} + \frac{\psi(L^{-1/3}(m-1))}{\psi(L^{-1/3}(m+1))} \\ &= -\frac{\bar{b}}{\lambda}m\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))} + L^{-1}\frac{\nu_m}{\psi(L^{-1/3}(m+1))}. \end{aligned} \quad (4.96)$$

We now let $\psi(x)$ be the specific complex solution (4.90), and try to control a complex solution of (4.1) such that $\varphi_{\ell_t+m} \simeq \psi(L^{-1/3}m)$. Information about the desired real solution can be read off easily, as we do at the end of the present section.

Let us introduce a complex quantity F_m by

$$\varphi_{\ell_t+m} = F_m\psi(L^{-1/3}m). \quad (4.97)$$

Then the Schrödinger equation (4.1) becomes

$$\begin{aligned} &F_{m+1}\psi(L^{-1/3}(m+1)) - 2F_m\psi(L^{-1/3}m) + F_{m-1}\psi(L^{-1/3}(m-1)) \\ &= -\beta_{\ell_t+m}F_m\psi(L^{-1/3}m). \end{aligned} \quad (4.98)$$

We divide this by $F_m\psi(L^{-1/3}(m+1))$to get

$$\begin{aligned} &\frac{F_{m+1}}{F_m} - 2\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))} + \frac{F_{m-1}}{F_m}\frac{\psi(L^{-1/3}(m-1))}{\psi(L^{-1/3}(m+1))} \\ &= -\beta_{\ell_t+m}\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))}. \end{aligned} \quad (4.99)$$

From (4.96) and (4.99), we get the following recursion equation for F_m.

$$\begin{aligned} \frac{F_{m+1}}{F_m} - 1 &= -\frac{\psi(L^{-1/3}(m-1))}{\psi(L^{-1/3}(m+1))}\left(\frac{F_{m-1}}{F_m} - 1\right) \\ &\quad - \left(\beta_{\ell_t+m} - \frac{\bar{b}}{\lambda}m\right)\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))} - \frac{\nu_m}{\psi(L^{-1/3}(m+1))}. \end{aligned} \quad (4.100)$$

We now use the asymptotic behavior (4.92) of $\psi(x)$ to see that

$$\begin{aligned} \left|\frac{\psi(L^{-1/3}(m-1))}{\psi(L^{-1/3}(m+1))}\right| &\le 1 + \text{const.}\left|\frac{\psi'(x)}{\psi(x)}\right| L^{-1/3} \\ &\le 1 + (c_9 + c_{10}x^{1/2})L^{-1/3} \\ &= 1 + c_9L^{-1/3} + c_{10}L^{-1/2}m^{1/2}, \end{aligned} \quad (4.101)$$

$$\left|\frac{\psi(L^{-1/3}m)}{\psi(L^{-1/3}(m+1))}\right| \le 1 + c_9 L^{-1/3} + c_{10} L^{-1/2} m^{1/2}, \tag{4.102}$$

and

$$\begin{aligned}
\left|\frac{\nu_m}{\psi(L^{-1/3}(m+1))}\right| &\le \text{const.}\left|\frac{\psi'''(x)}{\psi(x)}\right| \\
&\le c_{11} + c_{12} x^{3/2} \\
&= c_{11} + c_{12} L^{-1/2} m^{3/2}.
\end{aligned} \tag{4.103}$$

Let us define

$$G_m = \frac{F_m}{F_{m-1}} - 1. \tag{4.104}$$

By using the estimates (4.101), (4.102), (4.103) as well as (4.86), the recursion relation (4.100) reduces to

$$\begin{aligned}
|G_{m+1}| &\le \left(|G_m| + |G_m|^2\right)(1 + c_9 L^{-1/3} + c_{10} L^{-1/2} m^{1/2}) \\
&\quad + c_{13} L^{-1}(1 + c_9 L^{-1/3} + c_{10} L^{-1/2} m^{1/2}) \\
&\quad + c_{11} L^{-1} + c_{12} L^{-3/2} m^{3/2},
\end{aligned} \tag{4.105}$$

where we used

$$\left|\frac{F_{m-1}}{F_m} - 1\right| = \left|(G_m + 1)^{-1} - 1\right| \le |G_m| + |G_m|^2. \tag{4.106}$$

We now assume that $G_1 = 0$. Then we can estimate $|G_m|$ by repeatedly using (4.105). Let us assume $|G_m| \le \overline{G}$ holds for any m with $1 \le m \le c_2 L^{1/3}$ where the constant $\overline{G}$ will be determined later. Then (4.105) implies for any m with $1 \le m \le c_2 L^{1/3}$ that

$$\begin{aligned}
|G_m| &\le \sum_{j=1}^{m} \{|G_j| - |G_{j-1}|\} \\
&\le \overline{G}(c_2 c_9 + {c_2}^{3/2} c_{10}) \\
&\quad + \overline{G}^2 (c_2 L^{1/3} + c_2 c_9 + {c_2}^{3/2} c_{10}) \\
&\quad + c_2 c_{13} (L^{-2/3} + c_2 c_9 L^{-1} + {c_2}^{3/2} c_{10} L^{-1}) \\
&\quad + c_2 c_{11} L^{-2/3} + {c_2}^{5/2} c_{12} L^{-2/3}.
\end{aligned} \tag{4.107}$$

We now set

$$\overline{G} = c_{14} L^{-2/3}, \tag{4.108}$$

and substitute this relation into (4.107). We then find that, for sufficiently small (but L-independent) c_2, (4.107) reproduces $|G_m| \le \overline{G}$ with the same $\overline{G}$. This proves the upper bound

$$|G_m| \le c_{14} L^{-2/3}, \tag{4.109}$$

for m with $1 \le m \le c_2 L^{1/3}$.

Assuming $F_0 = 1$, we finally get

$$
\begin{aligned}
|F_m - 1| &= \left| \left(\prod_{j=1}^{m} \frac{F_j}{F_{j-1}} \right) - 1 \right| \\
&= \left| \left\{ \prod_{j=1}^{m} (1 + G_j) \right\} - 1 \right| \\
&\leq \exp[m c_{14} L^{-2/3}] - 1 \\
&\leq c_{15} L^{-1/3}, \qquad (4.110)
\end{aligned}
$$

for m with $1 \leq m \leq c_2 L^{1/3}$. Recalling (4.97), we have established the desired relation $\varphi_{\ell_t+m} \simeq \psi(L^{-1/3} m)$.

To control the desired real solution of (4.1), we only have to sum up the complex solution and its complex conjugate with appropriate complex weights. This proves

Lemma 7 *Let φ_ℓ be a real solution of (4.1). Then there is a complex constant A, and we have*

$$
\begin{aligned}
&\left| \varphi_\ell - \left\{ A\psi(L^{-1/3}(\ell - \ell_t)) + \overline{A\psi(L^{-1/3}(\ell - \ell_t))} \right\} \right| \\
&\leq 2c_{15} |A| \left| \psi(L^{-1/3}(\ell - \ell_t)) \right| L^{-1/3}, \qquad (4.111)
\end{aligned}
$$

for $\ell \in \tilde{I}_1 = \left\{ \ell_t, \ldots, \ell_t + [c_2 L^{1/3}] \right\}$, where $\psi(x)$ is explicitly given by (4.90).

We still have to treat the solution in the "classically accessible part" of the interval I_Ω, i.e., $\tilde{I}_\Omega = \left\{ \ell'_t - [c_2 L^{1/3}], \ldots, \ell'_t \right\}$. Since the analysis is exactly the same as that for $\tilde{I}_1$, we only present the final result.

Lemma 8 *Let φ_ℓ be a real solution of (4.1). Then there is a complex constant B, and we have*

$$
\begin{aligned}
&\left| \varphi_\ell - (-1)^\ell \left\{ B\psi(L^{-1/3}(\ell'_t - \ell)) + \overline{B\psi(L^{-1/3}(\ell'_t - \ell))} \right\} \right| \\
&\leq 2c_{15} |B| \left| \psi(L^{-1/3}(\ell'_t - \ell)) \right| L^{-1/3}, \qquad (4.112)
\end{aligned}
$$

for $\ell \in \tilde{I}_\Omega$, where $\psi(x)$ is explicitly given by (4.90).

4.6 Decay of the solution in the "classically inaccessible regions"

We now study the solution in the "classically inaccessible region", which is characterized by $|\alpha_\ell| > 1$. Since the Schrödinger equation (4.1) implies

$$
\varphi_\ell = -\frac{\varphi_{\ell-1} + \varphi_{\ell-1}}{2\alpha_\ell}, \qquad (4.113)
$$

we get a convexity inequality

$$
|\varphi_\ell| \leq \frac{|\varphi_{\ell-1}| + |\varphi_{\ell-1}|}{2|\alpha_\ell|} < \frac{|\varphi_{\ell-1}| + |\varphi_{\ell-1}|}{2}. \qquad (4.114)
$$

This means that $|\varphi_\ell|$ cannot take a local maximum.

Let us focus on the region $I'_\Omega = \{\ell'_{\mathrm{t}}+1,\ldots,nN\} \subset I_\Omega$. Then (4.114) means that $|\varphi_\ell|$ is decreasing because of the boundary condition $\varphi_{nN+1}=0$. Then (4.114) further implies

$$|\varphi_\ell| \le \frac{|\varphi_{\ell-1}|}{|\alpha_\ell|}, \tag{4.115}$$

and hence

$$|\varphi_\ell| \le |\varphi_{\ell'_{\mathrm{t}}}| \prod_{\ell'=\ell'_{\mathrm{t}}}^{\ell} |\alpha_{\ell'}|^{-1}. \tag{4.116}$$

We note that (4.42) implies

$$|\alpha_{\ell'}|^{-1} \le \left(1+\frac{g}{L}(\ell'-\ell'_{\mathrm{t}}) - \frac{ng}{L}\right)^{-1} \le \exp\left[-c_{16}(g/L)(\ell'-\ell'_{\mathrm{t}}-n)\right], \tag{4.117}$$

for $\ell'-\ell'_{\mathrm{t}} \le c_{17}L^{1-\mu}$ and any $\mu>0$. Recall that g is L-independent as in (4.37). Substituting (4.117) into (4.116), we get

$$|\varphi_\ell| \le |\varphi_{\ell'_{\mathrm{t}}}| c_{18} \exp\left[-c_{16}\frac{g}{L}(\ell'-\ell'_{\mathrm{t}})^2\right], \tag{4.118}$$

for $\ell'-\ell'_{\mathrm{t}} \le c_{17}L^{1-\mu}$. This means that $|\varphi_\ell|$ decays very rapidly in the "classically inaccessible region". For $\ell \ge c_{17}L^{1-\mu}$, we have

$$\frac{|\varphi_\ell|}{|\varphi_{\ell'_{\mathrm{t}}}|} \le c_{18}\exp\left[-c_{16}{c_{17}}^2\frac{g}{2}L^{1-2\mu}\right]. \tag{4.119}$$

In the most applications (see (3.15) and Lemma 5), we set $\mu=1/3$ in (4.119).

4.7 Boltzmann factor from the interior of the "classically accessible region"

We are now ready to prove the most important Lemma 2. We first treat the intervals I_ω with $\omega=\Gamma+1,\ldots,\Omega-\Gamma$. These intervals are located in the interior of the "classically accessible region", where the wave length of φ_ℓ is relatively short. In such situations, we must face possible "resonances" between the oscillation of $|\varphi_\ell|^2$ and the quasi periodic behavior of $\ell(j,k)$ (with j fixed and k varied), which (locally) destroys the desired "equal weighted" behavior. We will prove that such resonances are located in short intervals and do not have significant contributions.

Let I be one of I_ω with $\omega=\Gamma+1,\ldots,\Omega-\Gamma$. Our final goal is to evaluate the quantity $S_j/(\sum_{j'=1}^n S_{j'})$ for $j=1,2,\ldots,n$, where

$$S_j = \sum_{\ell\in I} \chi[j(\ell)=j]|\varphi_\ell|^2. \tag{4.120}$$

Because of the definition of the interval, we have

$$1-{\alpha_\ell}^2 \ge c_4 g L^{-\varepsilon}, \tag{4.121}$$

for any $\ell \in I$. (See the end of Section 4.4.) We also recall that the length of I satisfies

$$[c_5 L^{1-2\theta}/2] \le |I| \le [c_5 L^{1-2\theta}]. \tag{4.122}$$

To evaluate the sum S_j explicitly, we further decompose I into subintervals as

$$I = \bigcup_{q=1}^{Q} \hat{I}_q, \tag{4.123}$$

with each $\hat{I}_q$ having the length $|\hat{I}_q| = [c_{19} L^{\nu}]$, where $\nu > 0$ is another exponent to be determined later (to be 1/3). By $\hat{\ell}_q$ we denote the smallest element in $\hat{I}_q$. Consequently, we write

$$S_j = \sum_{q=1}^{Q} S_j^{(q)}, \tag{4.124}$$

with

$$S_j^{(q)} = \sum_{\ell \in \hat{I}_q} \chi[j(\ell) = j] |\varphi_\ell|^2. \tag{4.125}$$

Let $\ell \in \hat{I}_q$. We note that

$$\begin{aligned} \left| \frac{\sin \zeta_\ell}{\sin \zeta_{\hat{\ell}_q}} - 1 \right| &= \left| \frac{\sqrt{1 - {\alpha_\ell}^2}}{\sqrt{1 - {\alpha_{\hat{\ell}_q}}^2}} - 1 \right| \\ &\le \left(\max_{\ell \in \hat{I}_q} (1 - {\alpha_\ell}^2)^{-1} \right) (\alpha_\ell - \alpha_{\hat{\ell}_q}) \\ &\le \frac{c_{19}}{c_4} L^{\nu + \varepsilon - 1} \\ &\le \frac{c_{19}}{c_4} L^{-\eta}, \end{aligned} \tag{4.126}$$

where in the final line we used a new assumption on the exponents

$$\nu + \varepsilon - 1 \le -\eta. \tag{4.127}$$

We now use the estimate (4.126) and the approximate solution (4.83) to write the sum (4.125) more explicitly as

$$S_j^{(q)} = \frac{A^2}{\sin \zeta_{\hat{\ell}_q}} \sum_{\ell \in \hat{I}_q} \chi[j(\ell) = j] (\cos[Z_\ell + \xi])^2 + R_j^{(q)}, \tag{4.128}$$

where $R_j^{(q)}$ satisfies

$$\left| R_j^{(q)} \right| \le \frac{c_{20} A^2}{\sin \zeta_{\hat{\ell}_q}} |\hat{I}_q^{(j)}| L^{-\eta}, \tag{4.129}$$

where $\hat{I}_q^{(j)}$ is the subset of I_q with $j(\ell) = j$, and $|\hat{I}_q^{(j)}|$ denotes the number of its elements.

We now want to evaluate the sum over $\cos^2$ terms in (4.128). Let $\tilde{\zeta}_q = \zeta_{\hat{\ell}_q}$, and $\widetilde{Z}_q = Z_{\hat{\ell}_q - 1}$. Then we have

$$
\begin{aligned}
&\left|(\cos[Z_\ell + \xi])^2 - (\cos[\widetilde{Z}_q + \xi + \tilde{\zeta}_q(\ell - \hat{\ell}_q)])^2\right| \\
&\le 2 \max_{\ell \in \hat{I}_q} \left| Z_\ell - \left\{ \widetilde{Z}_q + \tilde{\zeta}_q(\ell - \hat{\ell}_q) \right\} \right| \\
&\le 2 \left(\max_{\ell \in \hat{I}_q} |\zeta_\ell - \tilde{\zeta}_q| \right) |\hat{I}_q| \\
&\le 2 \left(\max_{\ell \in \hat{I}_q} (1 - {\alpha_\ell}^2)^{-1/2} \right) \left| \alpha_\ell - \alpha_{\hat{\ell}_q} \right| |\hat{I}_q| \\
&\le 2 \sqrt{\frac{g}{c_4}} (c_{19})^2 L^{2\nu + (\varepsilon/2) - 1} \\
&\le 2 \sqrt{\frac{g}{c_4}} (c_{19})^2 L^{-\eta},
\end{aligned}
\tag{4.130}
$$

where the final line again makes use of the new assumption

$$
2\nu + \frac{\varepsilon}{2} - 1 \le \eta. \tag{4.131}
$$

We introduce a new constant $\tilde{\xi}_q = \widetilde{Z}_q + \xi - \tilde{\zeta}_q \hat{\ell}_q$. Then (4.130) essentially means that $(\cos[Z_\ell + \xi])^2 \simeq (\cos[\tilde{\zeta}_q \ell + \tilde{\xi}_q])^2$. So we are motivated study the sum

$$
\begin{aligned}
&\sum_{\ell \in \hat{I}_q} \chi[j(\ell) = j] (\cos[\tilde{\zeta}_q \ell + \tilde{\xi}_q])^2 \\
&= \frac{|\hat{I}_q^{(j)}|}{2} + \frac{1}{4} \sum_{\ell \in \hat{I}_q} \chi[j(\ell) = j] \left(e^{2i(\tilde{\zeta}_q \ell + \tilde{\xi}_q)} + e^{-2i(\tilde{\zeta}_q \ell + \tilde{\xi}_q)} \right),
\end{aligned}
\tag{4.132}
$$

which is a good approximation to the sum in (4.128). We expect the sum over oscillating exponential in (4.132) to be small, but this is not straightforward. Indeed, the sum is not at all small if a "resonance" between $\chi[j(\ell) = j]$ and the exponential term takes place. By using (4.32), we rewrite the sum of the first exponential term (times $e^{-2i\tilde{\xi}_q}$) as

$$
\begin{aligned}
&\sum_{\ell \in \hat{I}_q} \chi[j(\ell) = j] e^{2i\tilde{\zeta}_q \ell} \\
&= \sum_{k \text{s.t.} \ell(j,k) \in \hat{I}_q} \exp\left(2i\tilde{\zeta}_q \hat{\ell}_q + 2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j} k + \eta_{j,j'} \right] \right) \\
&= \sum_{p=0}^{k_{\max} - k_{\min}} \exp\left(2i\tilde{\zeta}_q \hat{\ell}_q + 2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j} p + \frac{\widetilde{M}_{j'}}{\widetilde{M}_j} k_{\min} + \eta_{j,j'} \right] \right),
\end{aligned}
\tag{4.133}
$$

where $[\cdots]$ is the Gauss symbol. The sum in the second line is over k such that $\ell(j,k) \in \hat{I}_q$ for the fixed j, and we denote this range of k as $\{k_{\min}, \ldots, k_{\max}\}$. We let $\bar{s} = [(k_{\max} -$

$k_{\min})/\widetilde{M}_j]$, and write $p = \widetilde{M}_j s + r$. Then the above sum becomes

$$\begin{aligned}
&= e^{2i\tilde{\zeta}_q\hat{\ell}_q} \sum_{s=0}^{\bar{s}-1} \sum_{r=0}^{\widetilde{M}_j-1} \exp\left(2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j}(\widetilde{M}_j s + r) + \tilde{\eta}_{j,j'}\right]\right) \\
&\quad + e^{2i\tilde{\zeta}_q\hat{\ell}_q} \sum_{p=\bar{s}\widetilde{M}_j}^{k_{\max}-k_{\min}} \exp\left(2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j}p + \tilde{\eta}_{j,j'}\right]\right) \\
&= e^{2i\tilde{\zeta}_q\hat{\ell}_q} \sum_{s=0}^{\bar{s}-1} \sum_{r=0}^{\widetilde{M}_j-1} \exp\left(2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left\{\widetilde{M}_{j'} s + \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j}r + \tilde{\eta}_{j,j'}\right]\right\}\right) \\
&\quad + (\text{the same second term}) \\
&= e^{2i\tilde{\zeta}_q\hat{\ell}_q} \frac{1 - e^{2i\tilde{\zeta}_q\widetilde{M}\bar{s}}}{1 - e^{2i\tilde{\zeta}_q\widetilde{M}}} \sum_{r=0}^{\widetilde{M}_j-1} \exp\left(2i\tilde{\zeta}_q \sum_{j'=1}^{n} \left[\frac{\widetilde{M}_{j'}}{\widetilde{M}_j}r + \tilde{\eta}_{j,j'}\right]\right) \\
&\quad + (\text{the same second term}),
\end{aligned} \tag{4.134}$$

where

$$\widetilde{M} = \sum_{j=1}^{n} \widetilde{M}_j. \tag{4.135}$$

By taking the absolute value of (4.133) and (4.134), we find

$$\begin{aligned}
\left|\sum_{\ell\in\hat{I}_q} \chi[j(\ell) = j] e^{2i\tilde{\zeta}_q\ell}\right| &\le \left(\frac{|\sin\tilde{\zeta}_q\widetilde{M}\bar{s}|}{|\sin\tilde{\zeta}_q\widetilde{M}|} + 1\right)\widetilde{M}_j \\
&\le \frac{2\widetilde{M}}{|\sin\tilde{\zeta}_q\widetilde{M}|}.
\end{aligned} \tag{4.136}$$

As we have anticipated, the right-hand side of (4.136) is usually small (compared with $|\hat{I}_q^{(j)}|$), but becomes large near the "resonance" points where $\tilde{\zeta}_q\widetilde{M}$ is equal to an integer multiple of 2π.

To control the final sum (4.124), we classify the subintervals $\hat{I}_1, \ldots, \hat{I}_Q$ into "good" ones and "bad" ones. A subinterval $\hat{I}_q$ is said to be good if

$$\frac{2\widetilde{M}}{|\sin\tilde{\zeta}_q\widetilde{M}|} \le c_{20}|\hat{I}_q|L^{-\eta}, \tag{4.137}$$

and to be bad otherwise. We want to know the possible number of the bad subintervals. First we note that the perfect resonance $\zeta_\ell\widetilde{M} = 2\pi \times (\text{integer})$ can take place in the whole interval I at most once, since ζ_ℓ varies at most by $O(L^{\nu+(\varepsilon/2)-1})$ within I. We suppose that there happens to be a perfect resonance (with ζ_{res}) within I, and see how many subintervals around it are "infected" and become bad. From (4.137) and that $|\hat{I}_q| = [c_{19}L^\nu]$, we get

$$|\tilde{\zeta}_q - \zeta_{\text{res}}| \ge \frac{L^{\eta-\nu}}{c_{20}c_{19}}, \tag{4.138}$$

for $\tilde{\zeta}_q$ corresponding to a good $\hat{I}_q$. This in turn means that the total number of the bad subintervals is bounded from above by

$$\begin{aligned}\frac{L^{\eta-\nu}}{c_{20}c_{19}}\left(\max_{\ell,\ell'\in I}|\zeta_\ell-\zeta_{\ell'}|\right)^{-1}Q &\leq \frac{L^{\eta-\nu}}{c_{20}c_{19}}(gc_5L^{-2\theta})^{-1}Q \\ &= \frac{1}{gc_5c_{20}c_{19}}L^{\eta-\nu+2\theta}Q \\ &\leq \frac{1}{gc_5c_{20}c_{19}}L^{-\eta}Q, \end{aligned} \tag{4.139}$$

where in the final line we assumed that

$$\eta-\nu+2\theta\leq-\eta. \tag{4.140}$$

To summarize, we have proved the following for the desired sum $S_j^{(q)}$ (4.125). When $\hat{I}_q$ is a "good" subinterval, we have

$$\left|S_j^{(q)}-\frac{A^2}{2\sin\zeta_{\hat{\ell}_q}}|\hat{I}_q^{(j)}|\right|\leq c_{21}\frac{A^2}{\sin\zeta_{\hat{\ell}_q}}|\hat{I}_q^{(j)}|L^{-\eta}. \tag{4.141}$$

When $\hat{I}_q$ is a "bad" subinterval, we have essentially no control on $S_j^{(q)}$, and can only say

$$\left|S_j^{(q)}\right|\leq c_{22}\frac{A^2}{\sin\zeta_{\hat{\ell}_q}}|\hat{I}_q^{(j)}|, \tag{4.142}$$

but we have the estimate (4.139) for the possible number of the "bad" intervals. Recalling (4.124), we sum up (4.141) and (4.142) with (4.139) in mind. We then get

$$\left|S_j-\tilde{S}_j\right|\leq c_{23}\tilde{S}_jL^{-\eta}, \tag{4.143}$$

with

$$\tilde{S}_j=\sum_{q=1}^{Q}\frac{A^2}{2\sin\zeta_{\hat{\ell}_q}}|\hat{I}_q^{(j)}|. \tag{4.144}$$

This immediately leads us to our goal (4.6) that

$$\left|\frac{S_j}{\sum_{j'=1}^n S_{j'}}-W_j\right|\leq c_1W_jL^{-\eta}, \tag{4.145}$$

with

$$W_j=\frac{|\hat{I}_q^{(j)}|}{\sum_{j'=1}^n|\hat{I}_q^{(j')}|}, \tag{4.146}$$

which is independent of q and is equal to (4.7).

4.8 Boltzmann factor from regions with long wave length

We still have to prove the main Lemma 2 for the interval I_ω with $\omega = 1, \ldots, \Gamma$ and $\omega = \Omega - \Gamma + 1, \ldots, \Omega$. In these intervals, the wave length of φ_ℓ is quite large, and the resonance effect (which made the estimates in Section 4.7 difficult) does not take place. The proof is rather straightforward, and we will be sketchy here.

In these intervals, we use one of the Lemmas 6, 7, or 8 to get controlled approximations for the solution φ_ℓ of the Schrödinger equation (4.1). In most of the situations, $|\varphi_\ell|$ can be treated essentially as a constant, and the estimate of (4.120) becomes as trivial as

$$S_j = \sum_{\ell \in I} \chi[j(\ell) = j] |\varphi_\ell|^2 \simeq |\varphi_\ell|^2 \sum_{\ell \in I} \chi[j(\ell) = j]. \tag{4.147}$$

The worst case that we have to worry about is when φ_ℓ changes its sign inside I. To investigate such a situation, we approximate $\varphi_\ell \simeq (\ell - \ell_{\min})$, and consider a small interval $I = \{\ell_{\min}, \ldots, \ell_{\max}\}$. The sum to be evaluated is

$$S_j = \sum_{\ell=\ell_{\min}}^{\ell_{\max}} \chi[j(\ell) = j](\ell - \ell_{\min})^2. \tag{4.148}$$

Though $j(\ell)$ may be a very complicated function of ℓ, (4.32) implies that it is (at least) a periodic function of ℓ with the period $\widetilde{M} = \sum_{j=1}^{n} \widetilde{M}_j$. Assuming $\ell_{\max} - \ell_{\min} = \bar{s}\widetilde{M}$, we evaluate for $r < \widetilde{M}$ the sum

$$\begin{aligned} \sum_{s=0}^{\bar{s}} (s\widetilde{M} + r)^2 &= \frac{\bar{s}(2\bar{s}+1)(\bar{s}+1)}{6} \widetilde{M}^2 + \bar{s}(\bar{s}+1)\widetilde{M}r + (\bar{s}+1)r^2 \\ &= \frac{\bar{s}(2\bar{s}+1)(\bar{s}+1)}{6} \widetilde{M}^2 (1 + O(1/\bar{s})), \end{aligned} \tag{4.149}$$

to see that the (unwanted) r-dependent terms are of order $O(1/\bar{s})$. Thus in order for $S_j / \sum_{j'=1}^{n} S_{j'}$ to become the desired Boltzmann factor with relative error $O(L^{-\eta})$, we must have that $\bar{s} \geq O(L^{\eta})$, and hence

$$\ell_{\max} - \ell_{\min} \geq \text{const.} L^{\eta}. \tag{4.150}$$

In the present situation, $\ell_{\max} - \ell_{\min}$ is determined by (the smaller of) the length of the interval and the wave length of the oscillation of φ_ℓ. Since the wave length in this region is longer than a constant times $L^{\varepsilon/2}$, the required conditions for the exponents are

$$\frac{\varepsilon}{2} \geq \eta, \quad \frac{1}{3} - \eta \geq \eta. \tag{4.151}$$

These guarantee the Lemma 2 for the desired intervals.

4.9 Determination of the exponents

In order to complete the lengthy proof of Lemma 2, we have to fix the values of the exponents η, ε, θ and ν so that several requirements are satisfied.

We now recall the requirements about the exponents appeared as (4.45), (4.79), (4.45), (4.81), (4.82), (4.127), (4.131), (4.140), and (4.151), which are

$$\begin{aligned} 1-\varepsilon &> \frac{1}{3}-\eta, \\ -2\theta+\varepsilon &\le 0, \\ \varepsilon &\le \frac{1}{2}, \\ -2\theta+\frac{\varepsilon}{2} &\le -\eta, \\ \nu+\varepsilon-1 &\le -\eta, \\ 2\nu+\frac{\varepsilon}{2}-1 &\le -\eta, \\ \eta-\nu+2\theta &\le -\eta, \\ \frac{\varepsilon}{2} &\ge \eta, \\ \frac{1}{3}-\eta &\ge \eta. \end{aligned} \tag{4.152}$$

As a solution which satisfies all of (4.152), we shall choose

$$\eta=\theta=\frac{1}{12}, \quad \nu=\frac{1}{3}, \quad \varepsilon=\frac{1}{6}. \tag{4.153}$$

This completes the proof.

5 General upper bounds for $|\varphi_{(j,k)}|$

In the main paper, we noted that the "hypothesis of equal weights for eigenstates" can be *partially* proved. Let me describe precise statements.

Recall that the "hypothesis of equal weights for eigenstates" consists of two parts;

1. $|\varphi_{(j,k)}|^2$ is negligible in the "classically inaccessible region."
2. $|\varphi_{(j,k)}|^2$ takes appreciable values all over in the "classically accessible region", and the value is essentially determined by a function f of the energy $E-(\varepsilon_j+B_k)$.

Clearly the second point is much more subtle. In fact if we take models with certain conservation laws, the second point is easily violated. The main point of our (unproven) hypothesis is that the above 2 holds in a general model which do not have any special symmetries or conservation laws.

On the other hand the first point is more universal, and may be stated for a large class of models rather easily. Here we prove two results which justify this second point. There can be various theorems under different assumptions. We here present two simple theorems, which are in some sense complimentary with each other.

We use the same notation as in the main paper, but now take general coupling Hamiltonian H', and denote its matrix elements as

$$V_{j,k;j',k'} = \langle \Psi_j \otimes \Gamma_k, H'\Psi_{j'} \otimes \Gamma_{k'} \rangle \,. \tag{5.1}$$

We also denote by $\mathcal{H}_\mathrm{S}$ and $\mathcal{H}_\mathrm{B}$ the Hilbert spaces for the subsystem and the bath.

As in the main paper, the the Schrödinger equation is

$$(H_\mathrm{S} \otimes \mathbf{1}_\mathrm{B} + \mathbf{1}_\mathrm{S} \otimes H_\mathrm{B} + H')\Phi = E\Phi. \tag{5.2}$$

Again expanding the eigenstate as

$$\Phi = \sum_{j=1}^{n} \sum_{k=1}^{N} \varphi_{(j,k)} \Psi_j \otimes \Gamma_k, \tag{5.3}$$

(5.2) is rewritten as

$$\{E - (\varepsilon_j + E_k)\}\, \varphi_{(j,k)} = \sum_{j',k'} V_{j,k;j',k'}\, \varphi_{(j',k')}, \tag{5.4}$$

for any $j = 1, \ldots, n$ and $k = 1, \ldots, N$.

We define

$$\lambda = \sup_{j,k} \sum_{j',k'} |V_{j,k;j',k'}|\,. \tag{5.5}$$

The first result is very simple.

Theorem 9 *Let a normalized state $\Phi \in \mathcal{H}_\mathrm{S} \otimes \mathcal{H}_\mathrm{B}$ satisfy (5.2). Then the coefficients $\varphi_{(j,k)}$ defined by (5.3) satisfy*

$$|\varphi_{(j,k)}| \le \frac{\lambda}{|E - (\varepsilon_j + B_k)|}. \tag{5.6}$$

Proof: From (5.4), we see that

$$\begin{aligned} |\varphi_{(j,k)}| &\le \frac{\sum_{j',k'} |V_{j,k;j',k'}|\, |\varphi_{(j',k')}|}{|E - (\varepsilon_j + B_k)|} \\ &\le \frac{\lambda}{|E - (\varepsilon_j + B_k)|}, \end{aligned} \tag{5.7}$$

where we noted $|\varphi_{(j,k)}| \le 1$ because Φ is normalized. ■

The bound (5.7) is very crude, but gives us the idea that $|\varphi_{(j,k)}|$ may be large for $|E - (\varepsilon_j + B_k)| \lesssim \lambda$, and is small for $|E - (\varepsilon_j + B_k)| \gg \lambda$.

To get stronger result, we further assume that there is a constant $D > 0$ such that $V_{j,k;j',k'} = 0$ if $|(\varepsilon_j + B_k) - (\varepsilon_{j'} + B_{k'})| > D$. In other words, the interaction Hamiltonian has no matrix elements between the basis states whose unperturbed energies differ by more than D. The assumption may hold for some interaction Hamiltonians which represent (near) elastic scattering, but not for some interactions. Under this assumption, we have the following.

Theorem 10 *Let a normalized state $\Phi \in \mathcal{H}_\mathrm{S} \otimes \mathcal{H}_\mathrm{B}$ satisfy (5.2). Then the coefficients $\varphi_{(j,k)}$ defined by (5.3) satisfy*

$$|\varphi_{(j,k)}| \le \frac{1}{n(j,k)!} \left(\frac{\lambda}{D}\right)^{n(j,k)}, \tag{5.8}$$

where the integer $n(j,k)$ is defined as

$$n(j,k) = \left[\frac{|E - (\varepsilon_j + B_k)|}{D} \right]. \tag{5.9}$$

Here $[\cdots]$ is the Gauss symbol.

Proof: The bound (5.8) (with the convention $0! = 1$) is trivial for j, k such that $n(j,k) = 0$. Assume (5.8) for all j', k' such that $n(j',k') \le n-1$. Take j, k such that $n(j,k) = n$. Then from (4.1) we have

$$\begin{aligned} |\varphi_{(j,k)}| &\le \frac{\lambda}{|E - (\varepsilon_j + B_k)|} \max_{(j',k')\mathrm{s.t.}|(\varepsilon_j + B_k) - (\varepsilon_{j'} + B_{k'})| \le D} |\varphi_{(j',k')}| \\ &\le \frac{\lambda}{nD} \frac{1}{(n-1)!} \left(\frac{\lambda}{D} \right)^{(n-1)} \\ &\le \frac{1}{n!} \left(\frac{\lambda}{D} \right)^{n}, \end{aligned} \tag{5.10}$$

which proves the desired bound. ■

The bound (5.8) shows that $|\varphi_{(j,k)}|$ actually decays very rapidly in the "classically inaccessible region."